

On the Convex Closure of the Graph of Modular Inversions

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Abstract

In this paper we give upper and lower bounds as well as a heuristic estimate on the number of vertices of the convex closure of the set

$$G_n = \{(a, b) : a, b \in \mathbb{Z}, ab \equiv 1 \pmod{n}, 1 \leq a, b \leq n-1\}.$$

The heuristic is based on an asymptotic formula of Rényi and Sulanke. After describing two algorithms to determine the convex closure, we

compare the numeric results with the heuristic estimate. The numeric results do not agree with the heuristic estimate — there are some interesting peculiarities for which we provide a heuristic explanation. We then describe some numerical work on the convex closure of the graph of random quadratic and cubic polynomials over \mathbb{Z}_n . In this case the numeric results are in much closer agreement with the heuristic, which strongly suggests that the the curve $xy = 1 \pmod{n}$ is “atypical”.

1 Introduction

Let G_n be the set

$$G_n = \{(a, b) : a, b \in \mathbb{Z}, ab \equiv 1 \pmod{n}, 1 \leq a, b \leq n-1\},$$

whose cardinality is given by the Euler function $\varphi(n)$. If we scale by a factor of $1/n$ we get the set of points $n^{-1}G_n$, which is uniformly distributed in the unit square. More precisely, if $\Omega \subseteq [0, 1]^2$ has piecewise smooth boundary and $N(\Omega, n)$ is the cardinality of the intersection $\Omega \cap n^{-1}G_n$, then it is natural to expect, and in fact can be proved by using the bounds of *Kloosterman sums*, that

$$\left| |\Omega| - \frac{N(\Omega, n)}{\varphi(n)} \right| \rightarrow 0 \quad \text{as } n \rightarrow \infty, \quad (1)$$

where $|\Omega|$ is the area of Ω . Figure 1, generated by MAPLE, illustrates this property.

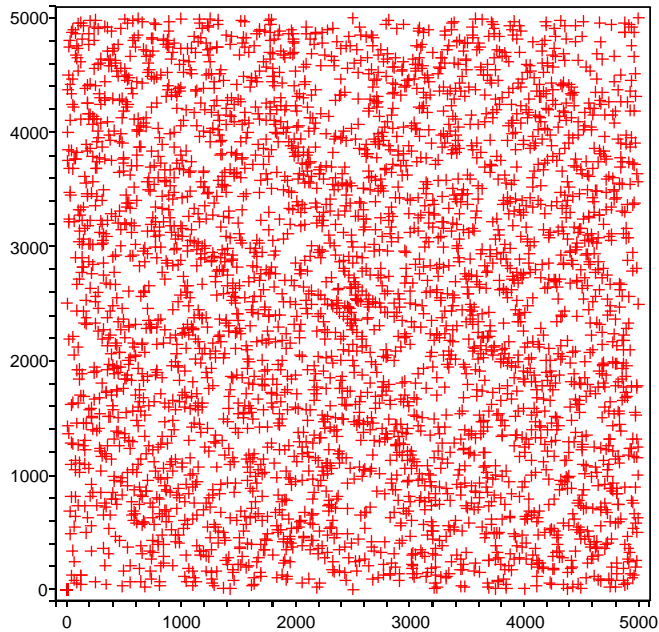


Fig. 1. The graph G_{5001}

Quantitative forms of (1) have been given in a number of works, see [3, 10, 25, 26, 27] and references therein. For example, it follows from more general results of [10] that for primes p ,

$$\left| |\Omega| - \frac{N(\Omega, p)}{p-1} \right| = O(p^{-1/4} \log p), \quad (2)$$

where the implied constant depends only on Ω .

Here we continue to study some geometric properties of the set G_n and in particular concentrate on the convex closure C_n of G_n . One of our questions of interest is the behavior of $v(n)$ and $V(N)$, where $v(n)$ denotes the number of vertices of C_n and $V(N)$ denotes the average,

$$V(N) = \frac{1}{N-1} \sum_{n=2}^N v(n).$$

We demonstrate that the theoretic and algorithmic study of $v(n)$ has surprising links with various areas of number theory, such as bounds of ex-

ponential sums, distribution of divisors of “typical” integers and integer factorisation. On the other hand, we present heuristic estimates $h(n)$ and $H(N)$ for $v(n)$ and $V(N)$, respectively. These heuristic estimates arise by viewing G_n as a set of points that are randomly distributed and then using the result of Rényi and Sulanke [17, Satz 1]. On comparing with our numeric results we see that although the heuristic prediction $H(N)$ gives an adequate idea about the type of growth of $V(N)$, there is a deviation which behaves quite regularly and thus probably reflects certain other hidden effects. We suggest some explanation. We also examine numerically some other interesting peculiarities in the behaviour of $v(n)$ which lead us to several open questions.

Finally, we present some numerical evidence suggesting that the above effects do not arise for sets of points on other curves which behave more like truly random sets of points, which makes the study of G_n even more interesting.

We note that some other geometric properties of the points of G_n have recently been considered in [20]. A survey of recent results about the distribution of points of G_n and more general sets corresponding to congruences of the type $ab \equiv \lambda \pmod{n}$ with some fixed λ , are given in [19].

2 Some Preliminary Observations

2.1 General structure of C_n

We begin with a simple (but useful) remark on two lines of symmetry of G_n .

Proposition 1. *The points of G_n are symmetrically distributed about the lines $y = x$ and $x + y = n$.*

Therefore, if $(a, b) \in G_n$, then its reflection in $y = x$, (b, a) , and its reflection in $x + y = n$, $(n - b, n - a)$, are elements of G_n . Consequently, (a, b) is a boundary point of C_n , if and only if (b, a) , $(n - b, n - a)$ and $(n - a, n - b)$ are boundary points of C_n .

Our next result shows that C_n is always a convex polygon with nonempty interior, except when $n = 2, 3, 4, 6, 8, 12, 24$.

Proposition 2. $|C_n| = 0$, if and only if $n = 2, 3, 4, 6, 8, 12$ or 24 .

Proof. This follows by observing that for these moduli all of the elements in \mathbb{Z}_n^* (that is, all units of the residue ring modulo n) have order 2. Consequently, for these moduli all of the elements of G_n lie on the line $y = x$. \square

From now on we typically exclude the cases $n = 2, 3, 4, 6, 8, 12$ and 24 .

2.2 Points in the triangle \mathcal{T}_n

By Proposition 1 we only need to know the vertices of C_n that lie in the triangle \mathcal{T}_n with vertices $(0, 0)$, $(0, n)$ and $(n/2, n/2)$, to determine C_n . We denote the vertices of C_n that lie in the triangle \mathcal{T}_n by

$$(a_0, b_0), (a_1, b_1), \dots, (a_s, b_s) \in C_n \cap \mathcal{T}_n,$$

where $a_0 < a_1 < \dots < a_s$.

Proposition 3. *We have the following:*

1. $(a_0, b_0) = (1, 1)$;
2. $a_i < b_i$ for $i = 1, \dots, s$;
3. $b_0 < b_1 < \dots < b_s$.
4. $b_i - a_i < b_{i+1} - a_{i+1}$ for $i = 0, \dots, s-1$.

Proof. Assertions 1 and 2 are clear. Assertions 3 and 4 follow from the following observation. The line through (a_i, b_i) and its symmetric counterpart $(n - b_i, n - a_i)$ intersects the line $x + y = n$ at the point $((n - b_i + a_i)/2, (n + b_i - a_i)/2)$. Since $a_i < a_{i+1}$ and (a_{i+1}, b_{i+1}) is a vertex of C_n , it follows that (a_{i+1}, b_{i+1}) must actually lie inside the smaller triangle with vertices (a_i, b_i) , $(a_i, n - a_i)$ and $((n - b_i + a_i)/2, (n + b_i - a_i)/2)$. \square

2.3 On the difference $b_s - a_s$

The inequalities in Proposition 3 may seem obvious, but they play a key role in our algorithms to compute the vertices of C_n . The vertex (a_s, b_s) has an important property. Let $M(n)$ denote the quantity

$$M(n) = \max \{|a - b| : 1 \leq a, b \leq n - 1 \text{ and } ab \equiv 1 \pmod{n}\}. \quad (3)$$

An immediate consequence of Proposition 3 is that

$$b_s - a_s = M(n).$$

The quantity $M(n)$ has been studied in [8, 15, 16]. It is shown in [16] that

$$n - M(n) \ll n^{3/4+o(1)}. \quad (4)$$

On the other hand, by [8, Theorem 3.1], for almost all n

$$n - M(n) \gg n^{1/2} (\log n)^{\delta/2} (\log \log n)^{3/4} f(n),$$

where

$$\delta = 1 - \frac{1 + \log \log 2}{\log 2} = 0.086071 \dots,$$

and $f(x)$ is any positive function tending monotonically to zero as $x \rightarrow \infty$. We recall that it has been proposed in [8, Conjecture 4.1] that the above bound is quite tight:

Conjecture 4. *For almost all n*

$$n - M(n) \ll n^{1/2} (\log n)^{\delta/2} (\log \log n)^{3/4} g(n),$$

where $g(x)$ is any function tending monotonically to ∞ as $x \rightarrow \infty$.

In support of Conjecture 4 we make the following observation. For a fixed $\varepsilon > 0$ define the set

$$\mathcal{N}(\varepsilon) = \{n \in \mathbb{N} : \exists d|(n-1) \text{ such that } n^{1/2-\varepsilon} \leq d \leq n^{1/2}\}.$$

By [11, Theorem 22] $\mathcal{N}(\varepsilon)$ has positive asymptotic density. Since

$$d \left(n - \frac{n-1}{d} \right) \equiv 1 \pmod{n},$$

we see that

$$n - M(n) \leq n - \left(n - \frac{n-1}{d} - d \right) = \frac{n-1}{d} + d \ll n^{1/2+\varepsilon},$$

for every n with this property. This immediately implies that for any $\varepsilon > 0$

$$n - M(n) \leq n^{1/2+\varepsilon}$$

for a set of n of positive density, which is a weaker form of what is assumed in Conjecture 4. In [8], one can also find more developed heuristic arguments supporting Conjecture 4.

We make one other remark about the vertex (a_s, b_s) . Following [22], we introduce the quantities

$$\rho_1(m) = \max_{d|m, d \leq \sqrt{m}} d \quad \text{and} \quad \rho_2(m) = \min_{d|m, d \geq \sqrt{m}} d.$$

We note that

$$a_s = \rho_1(kn - 1) \quad \text{and} \quad (n - b_s) = \rho_2(kn - 1),$$

where k is the integer such that $a_s(n - b_s) = kn - 1$.

2.4 Heuristic

Our heuristic attempt to approximate $v(n)$ makes use of a probabilistic model. Specifically, to view the points of $n^{-1}G_n$ as being randomly distributed in the unit square (which is supported by theoretic results of [3, 10, 25, 26, 27]) and then appeal to a result of Rényi and Sulanke [17, Satz 1]. Let \mathcal{R} be a convex polygon in the plane with r vertices and let P_i , $i = 1, \dots, n$, be n points chosen at random in \mathcal{R} with uniform distribution. Let X_n be the number of sides of the convex closure of the points P_i , and let $E(X_n)$ be the expectation of X_n . Then

$$E(X_n) = \frac{2}{3}r(\log n + \gamma) + c_{\mathcal{R}} + o(1), \quad (5)$$

where $\gamma = 0.577215\dots$ is the Euler constant, and $c_{\mathcal{R}}$ depends on \mathcal{R} and is maximal when \mathcal{R} is a regular r -gon or is affinely equivalent to a regular r -gon. In particular, for the unit square $\mathcal{R} = [0, 1]^2$ we have

$$c_{\mathcal{R}} = -\frac{8}{3} \log 2.$$

More precise results are given by Buchta and Reitzner [2], but they do not affect our arguments.

Using (5) with $r = 4$, it is plausible to conjecture that for most n

$$v(n) \approx h(n), \quad (6)$$

where

$$h(n) = \frac{8}{3}(\log \varphi(n) + \gamma - \log 2).$$

A portion of our work has been to generate numerical data to test this conjecture.

3 Bounds on $v(n)$

3.1 Lower Bounds

Here we give a lower bound on $v(n)$ in terms of the number of divisors function $\tau(n)$. We begin by establishing some notation and making a couple of pertinent observations.

For a fixed n , let us consider the curves $\alpha_j(n)$ and $\beta_j(n)$ defined by

$$\begin{aligned}\alpha_j(n) : \quad & x(n-y) = jn-1, \quad 1 \leq x \leq y \leq n-1, \\ \beta_j(n) : \quad & y(n-x) = jn-1, \quad 1 \leq y \leq x \leq n-1.\end{aligned}$$

A key observation used repeatedly is that for each point of G_n there is a j in the range $1, \dots, \lceil n/4 \rceil$ such that the point lies on the curve $\alpha_j(n)$ or $\beta_j(n)$. We denote the region bounded by the curves $\alpha_1(n)$ and $\beta_1(n)$ by \mathcal{R}_n . The next figure is an illustrative example. We note that the outermost curves are $\alpha_1(41), \beta_1(41)$.

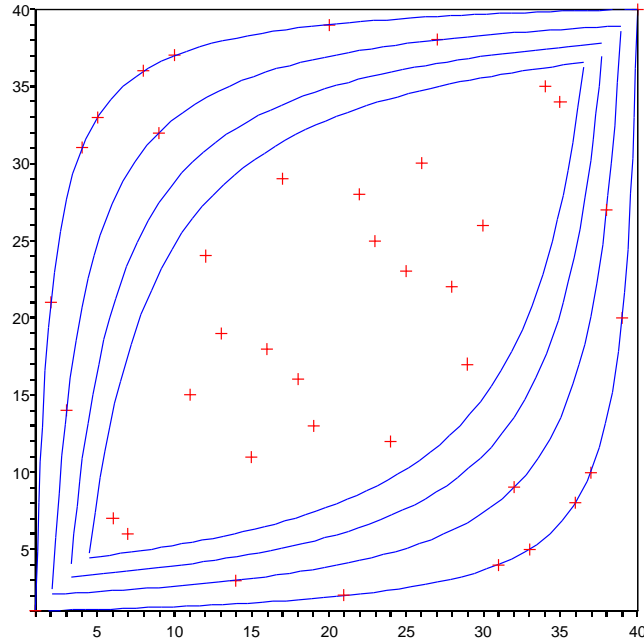


Fig. 2. The graph G_{41} and the curves $\alpha_j(41), \beta_j(41)$, $j = 1, 2, 3, 4$

For an integer $s \geq 1$ we denote

$$T(s) = \max_{i=1, \dots, \tau(s)-1} \frac{d_{i+1}}{d_i}$$

where $1 = d_1 < \dots < d_{\tau(s)} = s$ are the positive divisors of s .

Clearly,

$$T(s) \leq P(s), \quad (7)$$

where $P(s)$ denotes the largest prime divisor of s .

Let D_n be the convex closure of the points $(d_i, n - (n-1)/d_i), (n - (n-1)/d_i, d_i)$, for $i = 1, \dots, \tau(n-1)$. Clearly, we have the inclusions $D_n \subseteq C_n \subseteq \mathcal{R}_n$. We remark that if $n-1$ is prime, the set D_n is simply the line segment connecting the points $(1, 1)$ and $(n-1, n-1)$.

The purpose of our next proposition is to give a criterion to determine which of the $\alpha_j(n)$, $2 \leq j \leq \lceil n/4 \rceil$, lie strictly in the interior of D_n , and hence strictly in the interior of C_n . We denote by Γ_n the set of boundary points (x, y) of D_n such that $y \geq x$, that is, $\Gamma_n = \{(x, y) : (x, y) \in \partial D_n, y \geq x\}$.

Proposition 5. *Let $1 = d_1 < \dots < d_{\tau(n-1)} = n-1$ be the positive divisors of $n-1$. Then, for any integer $m \geq 2$,*

$$\Gamma_n \cap \alpha_m(n) = \emptyset \quad \Leftrightarrow \quad \frac{d_{i+1}}{d_i} + \frac{d_i}{d_{i+1}} < 4m - 2 + \frac{4(m-1)}{n-1}, \quad i = 1, \dots, \tau(n-1)-1.$$

Proof. This is a routine computation and so we only sketch an outline. The polygonal curve Γ_n is the union of line segments

$$L_i : \quad (1-t)(d_i, n - (n-1)/d_i) + t(d_{i+1}, n - (n-1)/d_{i+1}), \quad 0 \leq t \leq 1,$$

with $i = 1, \dots, (\tau(n-1)-1)$. Now $L_i \cap \alpha_m(n) = \emptyset$ if and only if the quadratic equation in t

$$(d_{i+1} - d_i) \left(\frac{n-1}{d_{i+1}} - \frac{n-1}{d_i} \right) t^2 - (d_{i+1} - d_i) \left(\frac{n-1}{d_{i+1}} - \frac{n-1}{d_i} \right) t + (1-m)n = 0$$

has no real solutions. □

A useful consequence of Proposition 5 is that if

$$m \geq \left\lfloor \frac{T(n-1) + 3}{4} \right\rfloor, \quad (8)$$

with $m \in \mathbb{Z}$ and $m \geq 2$, then $\Gamma_n \cap \alpha_m(n) = \emptyset$.

Theorem 6. *For all $n \geq 2$,*

$$v(n) \geq 2(\tau(n-1) - 1),$$

and for sufficiently large x ,

$$\#\{n \leq x : v(n) = 2(\tau(n-1) - 1)\} \gg \frac{x}{\log x}.$$

Proof. Since $C_n \subseteq \mathcal{R}_n$, any $(x, y) \in G_n \cap (\alpha_1(n) \cup \beta_1(n))$ is a vertex of C_n , and either x or y is a divisor of $(n-1)$. Therefore, $v(n) \geq 2(\tau(n-1) - 1)$.

By (8) we have $\Gamma_n \cap \alpha_2(n) = \emptyset$ for every n with $T(n-1) \leq 5$. Consequently, for such n , all of the vertices of C_n lie on $\alpha_1(n) \cup \beta_1(n)$ and thus $v(n) = 2(\tau(n-1) - 1)$. On the other hand, by [18, Theorem 1], we know that for any fixed t and sufficiently large x ,

$$\#\{n \leq x : T(n-1) \leq t\} \asymp \frac{x \log t}{\log x}$$

Applying this result with $t = 5$ we conclude the proof. \square

It is easy to construct explicit examples of n with $v(n) = 2(\tau(n-1) - 1)$. For instance it follows from (7) and (8) that this holds for $n = 2^r 3^s 5^t + 1$, where r, s, t are non-negative integers.

Since for any $\delta > 0$ we have

$$\limsup_{k \rightarrow \infty} \tau(k) 2^{-(1-\delta) \log k / \log \log k} = \infty$$

(see [12, Theorem 317]), the same holds true for $v(n)$, and so we can infer that the heuristic estimate (6) is sometimes exponentially smaller than $v(n)$.

Corollary 7. *For any $\delta > 0$*

$$\limsup_{n \rightarrow \infty} v(n) 2^{-3/8(1-\delta)h(n)/\log h(n)} = \infty.$$

We have that $v(n) \geq 2(\tau(n-1) - 1)$, and it is natural to ask when does one have strict inequality. Our next result gives a partial answer to this question. Specifically, we exhibit a set of positive density for which we have strict inequality. Furthermore, if we assume Conjecture 4 then we have strict inequality for almost all n .

Theorem 8. *The strict inequality*

$$v(n) > 2(\tau(n-1) - 1)$$

holds

i. for a set of n of positive density.

ii. for almost all n , provided that for almost all n we have $n - M(n) \leq n^{1/2+o(1)}$.

Proof. *i.* Let

$$\mathcal{E}(x) = \{n \leq x : v(n) = 2(\tau(n-1) - 1)\},$$

and

$$\mathcal{I}(x) = \{n \leq x : a_s(n - b_s) = n - 1\}.$$

It is important to note that the values of s , a_s and b_s all depend on n . We remind the reader of the following properties of the point (a_s, b_s) used in the proof below. It is the highest vertex of C_n that lies on or below the line $x + y = n$; $M(n) = b_s - a_s$ and $a_s \leq n - b_s$. Clearly, $\mathcal{E}(x) \subseteq \mathcal{I}(x)$.

The set of positive density we have in mind is

$$\mathcal{A}(x) = \{n \leq x : \exists p \text{ prime with } p|(n-1) \text{ and } p \geq x^{0.76}\}.$$

Using *Mertens's formula*, (see [12, Theorem 427]), we get that

$$\#\mathcal{A}(x) = \sum_{x^{0.76} \leq p \leq x} \left\lfloor \frac{x-1}{p} \right\rfloor \sim (\log(25/19))x.$$

Since $\mathcal{E}(x) \subseteq \mathcal{I}(x)$, in order to prove

$$\lim_{x \rightarrow \infty} \frac{\#(\mathcal{A}(x) \cap \mathcal{E}(x))}{x} = 0$$

it is enough to prove that

$$\lim_{x \rightarrow \infty} \frac{\#(\mathcal{A}(x) \cap \mathcal{I}(x))}{x} = 0.$$

We now write $\mathcal{I}(x)$ as the disjoint union of the two sets $\mathcal{I}_1(x)$, $\mathcal{I}_2(x)$, where

$$\begin{aligned}\mathcal{I}_1(x) &= \{n \in \mathcal{I}(x) : n - b_s \leq x^{0.24}\}, \\ \mathcal{I}_2(x) &= \{n \in \mathcal{I}(x) : x^{0.24} < n - b_s < x^{0.76}\}.\end{aligned}$$

The exponent values, 0.24 and 0.76, come from the asymptotic $n - M(n) \leq n^{3/4+o(1)}$ that we mentioned earlier. Since $\#\mathcal{I}_1(x) \leq x^{0.48}$ and for x large $\mathcal{A}(x) \cap \mathcal{I}_2(x) = \emptyset$, it follows that for large x

$$\#(\mathcal{A}(x) \cap \mathcal{I}(x)) = \#(\mathcal{A}(x) \cap \mathcal{I}_1(x)) + \#(\mathcal{A}(x) \cap \mathcal{I}_2(x)) \leq \#\mathcal{I}_1(x) = o(x).$$

ii. We now prove the following conditional statement. If for almost all n , $n - M(n) \leq n^{1/2}g(n)$ with some function $g(n) = n^{o(1)}$, then $\#\mathcal{I}(x) = o(x)$.

Without loss of generality we may assume that $g(n)$ is monotonically increasing. This time we write $\mathcal{I}(x)$ as the disjoint union of three sets, $\mathcal{J}_1(x)$, $\mathcal{J}_2(x)$ and $\mathcal{J}_3(x)$ where

$$\begin{aligned}\mathcal{J}_1(x) &= \left\{n \in \mathcal{I}(x) : n - b_s \leq \frac{\sqrt{x}}{g(x)}\right\}, \\ \mathcal{J}_2(x) &= \left\{n \in \mathcal{I}(x) : \frac{\sqrt{x}}{g(x)} < n - b_s \leq \sqrt{x}g(x)\right\}, \\ \mathcal{J}_3(x) &= \{n \in \mathcal{I}(x) : \sqrt{x}g(x) < n - b_s < x^{0.76}\}.\end{aligned}$$

Now $\#\mathcal{J}_1(x) \leq xg(x)^{-2} = o(x)$, and by our assumption we also have $\#\mathcal{J}_3(x) = o(x)$. So to conclude we need to show that $\#\mathcal{J}_2(x) = o(x)$. This follows by the following observation. Let

$$H(x, y, z) = \{n \leq x : \exists d|n \text{ with } y < d \leq z\}.$$

Then

$$\#\mathcal{J}_2(x) \leq H\left(x, \sqrt{x}/g(x), \sqrt{x}g(x)\right),$$

and by [7, Theorem 1],

$$H\left(x, \sqrt{x}/g(x), \sqrt{x}g(x)\right) = o(x)$$

which concludes the proof. \square

We remark that the assumption of Theorem 8 (ii) is weaker than Conjecture 4. The bound of Conjecture 4 probably holds for almost all primes. This would then imply that

$$v(p) > 2(\tau(p-1) - 1)$$

for almost all primes p . On the other hand, it is reasonable to expect that there are infinitely many primes of the form $n = 2^r 3^s 5^t + 1$ (in fact even of the form $p = 3 \cdot 2^r + 1$), and therefore equality would occur infinitely often, as well. We conclude this section by proving that $v(n)$ can be substantially larger than $\tau(n-1)$.

Theorem 9. *There is an infinite sequence of integers n_j with*

$$v(n_j) \geq \exp\left(\left(\frac{2 \log 2}{11} + o(1)\right) \frac{\log n_j}{\log \log n_j}\right) \quad \text{and} \quad \tau(n_j - 1) = 2.$$

Proof. Let n be a shifted prime, that is, $n = p + 1$, where p is prime. We first show that for such integers,

$$v(n) = v(p+1) \geq 2(\tau(2p+1) - 3).$$

Let ℓ be the line through $(1, 1)$ which is tangent to $\alpha_2(n)$. Since $(1, 1)$ and (p, p) are the only points of G_n on $\alpha_1(n)$, all of the points of G_n lie on or below ℓ . A straightforward calculation shows that ℓ meets $\alpha_2(n)$ at the point (x, y) where the x -coordinate is

$$x = \frac{1}{1 - ((p+1)/(2p+1))^{1/2}} < 4.$$

Hence every divisor d of $2p+1$, with $3 < d < (2p+1)/3$, gives rise to a vertex on $\alpha_2(n)$. Consequently the number of vertices on $\alpha_2(n)$ is at least $\tau(2p+1) - 4$. By symmetry there are an equal number of vertices on $\beta_2(n)$, and since $(1, 1)$ and (p, p) are also vertices of C_n , we obtain the desired inequality.

We now let Q_j denote the product of first j odd primes and set p_j to be the smallest prime satisfying the congruence $2p_j \equiv -1 \pmod{Q_j}$. By the Prime Number Theorem $\log Q_j \sim j \log j$, and by Heath-Brown's [13] version of Linnik's theorem we have $p_j < cQ_j^{11/2}$, for an absolute constant $c \geq 1$. On combining $p_j < cQ_j^{11/2}$ with the asymptotic $\log Q_j \sim j \log j$ we obtain

$$\tau(2p_j + 1) \geq \tau(Q_j) = 2^j \geq \exp\left(\left(\frac{2 \log 2}{11} + o(1)\right) \frac{\log p_j}{\log \log p_j}\right).$$

Setting $n_j = p_j + 1$ we conclude the proof. \square

In particular, we see from Theorem 9 that

$$\limsup_{n \rightarrow \infty} \frac{\log v(n)}{\log \tau(n-1)} = \infty.$$

Furthermore we can replace the terms $\log v(n)$ and $\log \tau(n-1)$ by the k -fold iteration of the logarithm for any $k \in \mathbb{N}$. Unfortunately, we do not see any approaches to the following.

Conjecture 10. *We have*

$$\liminf_{n \rightarrow \infty} v(n) = \infty.$$

3.2 Upper Bounds

Theorem 11. *For $n \rightarrow \infty$,*

$$v(n) \leq n^{3/4+o(1)}.$$

Proof. In Section 2.2, we labelled the highest vertex of C_n in the triangle \mathcal{T}_n by (a_s, b_s) . Trivially, $s \leq a_s$ and $a_s \leq n - b_s$. Hence

$$v(n) \leq 4s + 2 \leq 4a_s + 2 \leq 2(n - b_s + a_s + 1) = 2(n - M(n) + 1),$$

and the bound (4) concludes the proof. \square

Most certainly the bound of Theorem 11 is not tight. If we assume Conjecture 4, then

$$v(n) \leq n^{1/2+o(1)}$$

for almost all n . This still seems too high and the actual order of $v(n)$ is almost certainly much smaller. A different upper bound for $v(n)$ can be derived from (8). For integers n where $n-1$ has only small prime factors, this upper bound is significantly better than Theorem 11.

Theorem 12. *For $n \rightarrow \infty$,*

$$v(n) \leq T(n-1)n^{o(1)}.$$

Proof. From (8) we see that only points from the curves $\alpha_j(n)$ and $\beta_j(n)$ where,

$$j \leq m_n = \left\lfloor \frac{T(n-1) + 3}{4} \right\rfloor,$$

contribute to $v(n)$. Since every curve $\alpha_j(n)$, $\beta_j(n)$ contains at most $\tau(jn-1)$ points of G_n we derive

$$v(n) \leq \sum_{j=1}^{m_n} 2\tau(jn-1).$$

We conclude by invoking the asymptotic inequality $\tau(r) \ll r^{o(1)}$, see [12, Theorem 315]. \square

4 Computing C_n

4.1 Systematic search algorithm

We now describe a deterministic algorithm to construct the vertices of C_n that lie in the triangle \mathcal{T}_n . It is a variant of the famous algorithm of Graham [9] known as GRAHAM SCAN. The main virtue of our algorithm, as opposed to using some other convex closure algorithms, is that we do not need to generate and store all of the points of G_n before determining the convex closure. Instead, we generate the points one by one, discard most of them along the way, and halt in a reasonable amount of time.

Algorithm 13. 1. Set $a_0 := 1; b_0 := 1$.

2. For $i = 0, 1, \dots$:

(a) Set $a_{i+1} :=$ to be the smallest integer $a \in \mathbb{Z}_n^*$ satisfying the inequalities

$$a_i < a \leq \frac{n + a_i - b_i}{2} \quad \text{and} \quad b_i - a_i < a^{-1} - a.$$

If either of the above conditions cannot be met the algorithm terminates.

(b) Set $b_{i+1} := a^{-1}$.

(c) *Convexity check:*

- i. If $i = 1$ goto Step 2(a).
- ii. If $i \geq 2$ and the angle between the points $(a_{i-1}, b_{i-1}), (a_i, b_i)$ and (a_{i+1}, b_{i+1}) is reflex then return to Step 2(a), otherwise discard the point (a_i, b_i) and set

$$a_i := a_{i+1}, \quad b_i := b_{i+1}, \quad i := i - 1$$

and return to Step 2(c).

We note that the inequalities in Step 2a are motivated by Proposition 3. Clearly, Algorithm 13 is deterministic and it immediately follows from (4) that its complexity is $O(n^{3/4+o(1)})$.

4.2 Factorisation based algorithm

The observation that the points in $G_n \cap \alpha_1(n)$ are vertices of C_n combined with (8) allows us to devise a variation on Algorithm 13. The idea is to first use factorisation to create a smaller input set and then run the algorithm.

Let \mathcal{P}_n be the polygonal region with vertices

$$(1, n-1), (1, 1), (d_1, n - (n-1)/d_1), \dots, (d_k, n - (n-1)/d_k), \\ ((n-1)/d_k + d_k)/2, n - ((n-1)/d_k + d_k)/2, (\sqrt{n-1}, n - \sqrt{n-1}),$$

where $1 = d_0 < d_1 < \dots < d_k$ are the factors of $n-1$ which are less than or equal to $\sqrt{n-1}$. Since the vertices of C_n can only lie on the curves $\alpha_j(n)$, $\beta_j(n)$ where

$$j \leq m_n = \left\lfloor \frac{T(n-1) + 3}{4} \right\rfloor,$$

we need only determine which of the points of the union

$$U_n = \bigcup_{j=1}^{m_n} S_{j,n},$$

are vertices of C_n , where $S_{j,n} = \alpha_j(n) \cap G_n \cap \mathcal{P}_n$. It is useful to keep in mind that

$$\#U_n \leq \sum_{j=1}^{m_n} \#S_{j,n} \leq \sum_{j=1}^{m_n} \tau(jn-1) = m_n n^{o(1)},$$

see [12, Theorem 315]. We now apply the following algorithm.

Algorithm 14.

1. *Factorization:*

- (a) Find all of the factors $1 = d_0 < d_1 < \dots < d_k \leq \sqrt{n-1}$ of $n-1$.
- (b) Set $S_1 := \{(1, 1), (d_1, n - (n-1)/d_1), \dots, (d_k, n - (n-1)/d_k)\}$.
- (c) Compute $t := T(n-1)$.
- (d) Set $m_n := \lfloor (t+3)/4 \rfloor$.
- (e) For $j = 2, \dots, m_n$, factor $jn-1$ and construct the set $S_{j,n}$.
- (f) Set $U_n := \cup_{j=1}^{m_n} S_{j,n}$.

2. *Determining the vertices:*

- (a) Order the points of U_n by increasing first co-ordinate.
- (b) Apply the appropriate versions of Steps 2a and 2c of Algorithm 13 to the elements of U_n .

The complexity of Algorithm 14 depends on the type of algorithm we use for the factorisation step. If we use any subexponential probabilistic factorisation algorithm which runs in time $n^{o(1)}$, (see [4, Chapter 6]), then the complexity of Step 1 of Algorithm 14 is at most

$$\#U_n n^{o(1)} = m_n n^{o(1)}.$$

Furthermore, the complexity of Step 2 of Algorithm 14 is of the same form as well. So the overall complexity of Algorithm 14 is at most

$$m_n n^{o(1)} = T(n-1) n^{o(1)}.$$

This is lower than that of Algorithm 13 if $T(n-1) \leq n^{3/4}$. For any fixed $\lambda \geq 0$ the proportion of the positive integers k with $T(k) \leq k^\lambda$ is given by a certain continuous function $\psi(\lambda) > 0$, see [23]. Using [18, Corollary A] we conclude that

$$\psi(3/4) = \int_0^{7/8} \rho\left(\frac{1}{x} - 1\right) \frac{dx}{x} = \int_{1/7}^{\infty} \rho(y) \frac{dy}{1+y} = 0.866468\dots$$

where $\rho(u)$ is the *Dickman function*, see [5] or [24, Section III.5.4]. Thus the proportion of the positive integers n with $T(n-1) \leq n^{3/4}$ is $\psi(3/4) =$

0.866468... (The bound in Step 1d of Algorithm 14 is certainly not tight. It can probably be replaced by a bound of order $n^{o(1)}$ or even possibly a power of $\log n$, but unfortunately we have not been able to prove such a result.)

On the other hand, if we use a deterministic factoring algorithm in Step 1, then Algorithm 14 is of complexity at most

$$m_n(m_n n)^{1/4+o(1)} = T(n-1)^{5/4} n^{1/4+o(1)}$$

unconditionally, and of complexity at most

$$m_n(m_n n)^{1/5+o(1)} = T(n-1)^{6/5} n^{1/5+o(1)}$$

under the *Extended Riemann Hypothesis*, see [4, Section 6.3]. Accordingly, this is better than Algorithm 13 for $T(n-1) < n^{2/5}$ and $T(n-1) < n^{11/24}$ respectively. The corresponding proportions of the positive integers, n , satisfying these inequalities are $\psi(2/5)$ and $\psi(11/24)$. Since [18, Corollary A] expresses both $\psi(2/5)$ and $\psi(11/24)$ as double integrals, it is easier to compute $\psi(3/4)$ than either of these two values.

5 Computational Results

5.1 Expected value of $V(N)$

Let

$$\eta = \sum_p \frac{\log(1 - 1/p)}{p} = -0.580058 \dots,$$

where the sum runs over all prime numbers p . Surprisingly enough, this quantity has already appeared in various, seemingly unrelated number theoretic questions, see [6, page 122].

Proposition 15. *We have,*

$$\frac{1}{N} \sum_{n=1}^N \log \varphi(n) = \log N + \eta - 1 + O\left(\frac{\log \log N}{N}\right).$$

Proof. Obviously,

$$\frac{1}{N} \sum_{n=1}^N \log \varphi(n) = \frac{1}{N} \sum_{n=1}^N \log n + \frac{1}{N} \sum_{n=1}^N \sum_{p|n} \log(1 - 1/p),$$

where the last sum is taken over prime divisors $p|n$. The first sum on the right-hand side is $\log N - 1 + o(1)$ by *Stirling's formula*. By changing the order of summation in the second sum, we derive

$$\begin{aligned}
\frac{1}{N} \sum_{n=1}^N \sum_{p|n} \log(1 - 1/p) &= \frac{1}{N} \sum_{p \leq N} \log(1 - 1/p) \sum_{\substack{n \leq N \\ p|n}} 1 \\
&= \frac{1}{N} \sum_{p \leq N} \log(1 - 1/p) \left(\frac{N}{p} + O(1) \right) \\
&= \sum_{p \leq N} \frac{\log(1 - 1/p)}{p} + O \left(\frac{1}{N} \sum_{p \leq N} \frac{1}{p} \right) \\
&= \sum_{p \leq N} \frac{\log(1 - 1/p)}{p} + O \left(\frac{\log \log N}{N} \right),
\end{aligned}$$

where the last step follows by *Mertens's formula*, see [12, Theorem 427]. Observing that

$$\sum_{p \leq N} \frac{\log(1 - 1/p)}{p} = \eta - \sum_{p > N} \frac{\log(1 - 1/p)}{p} = \eta + O \left(\frac{1}{N} \right),$$

we conclude our proof. \square

Combining heuristic (6) with Proposition 15 for the average $V(N)$, we get the heuristic $V(N) \sim H(N)$, where

$$H(N) = \frac{8}{3}(\log N + \gamma + \eta - 1 - \log 2) \approx 2.66666 \cdot \log N - 4.52264.$$

In Figure 3 we compare the graph of $V(N)$, $H(N)$ and the least squares approximation

$$L(N) = 3.551166 \cdot \log N - 9.610899 \tag{9}$$

to $V(N)$, where N ranges over the interval $[2, 5770001]$. The values of $V(N)$ are represented by diamonds along the graph of $L(N)$, while $H(N)$ is the lower curve.

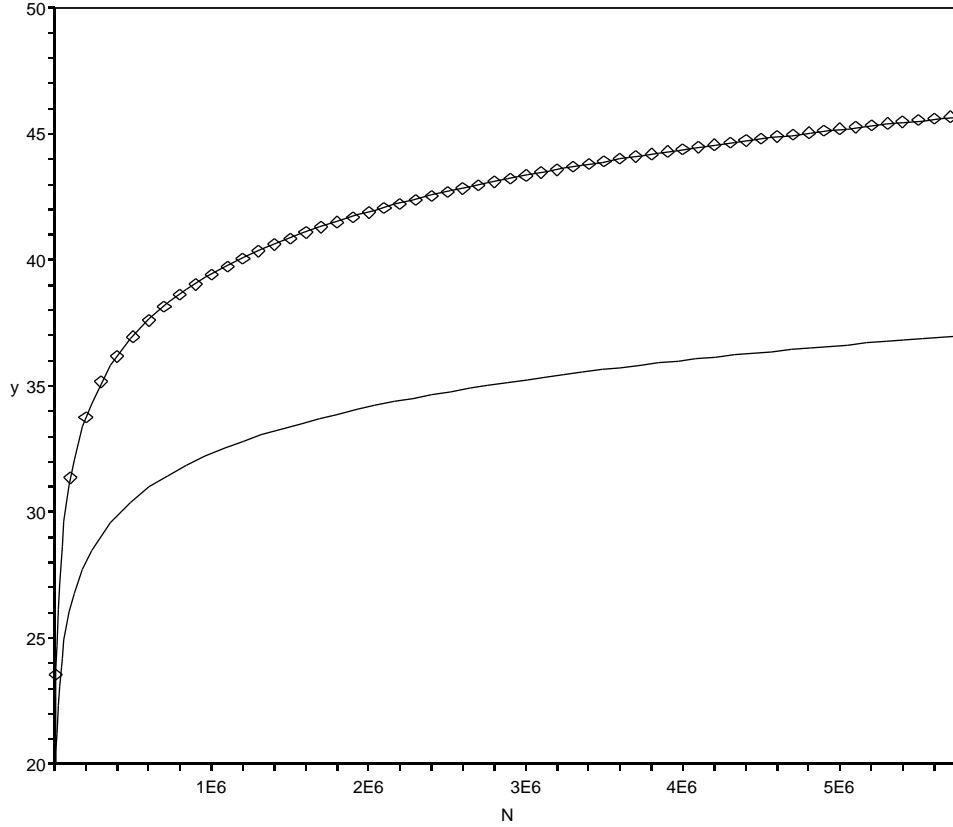


Fig. 3. $V(N)$, $H(N)$, and $L(N)$ for $2 \leq N \leq 5770001$

We see that although $V(N)$ behaves like a logarithmic function and thus resembles $H(N)$, they clearly deviate. This deviation seems to be of regular nature and suggests that there should be a natural explanation for this behaviour of $V(N)$. In an attempt to understand this we computed $v(n)$, $h(n)$ and $\tau(n-1)$ for 50000 random integers in the interval $[10^6, 10^8]$, and did some comparisons. We present the individual data in the histograms in Figures 4 and 5, and the comparisons in Figures 6, 7, 8, 9 and 11. In several histograms the extreme values on the right are not visible. Hence, for visual clarity we have truncated them on the right. Under each histogram we state in the caption the minimum value, the maximum value and the number of values that are not shown.

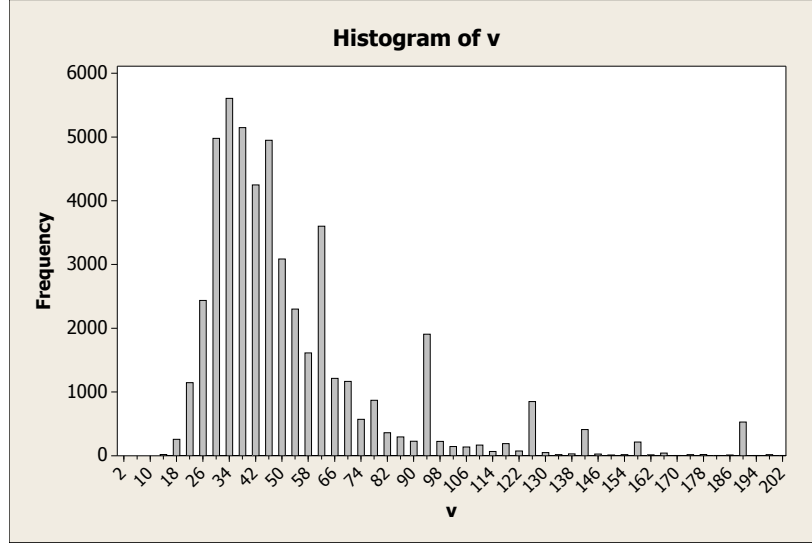


Fig. 4. Frequency histogram of $v(n)$
min = 14, max = 766 (645 values omitted)

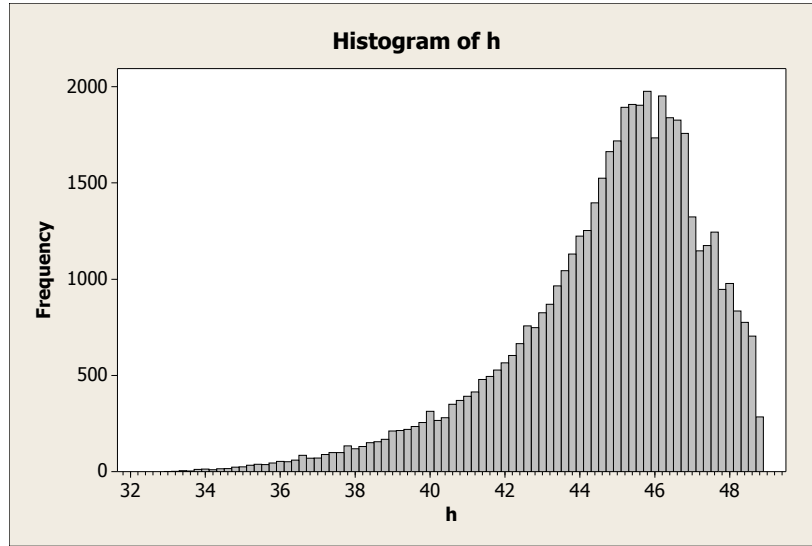


Fig. 5. Frequency histogram of $h(n)$
min = 33.01, max = 48.81

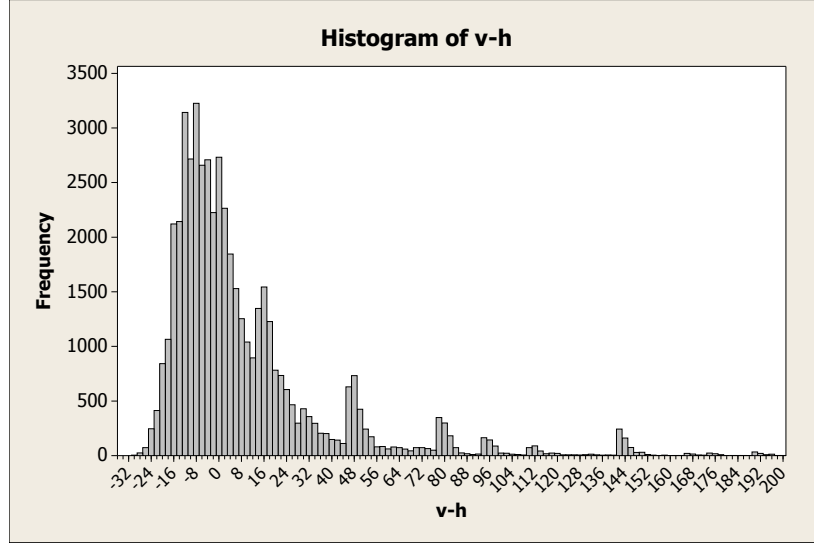


Fig. 6. Frequency histogram of $(v - h)$
min = -29.93 , max = 714.41 (458 values omitted)

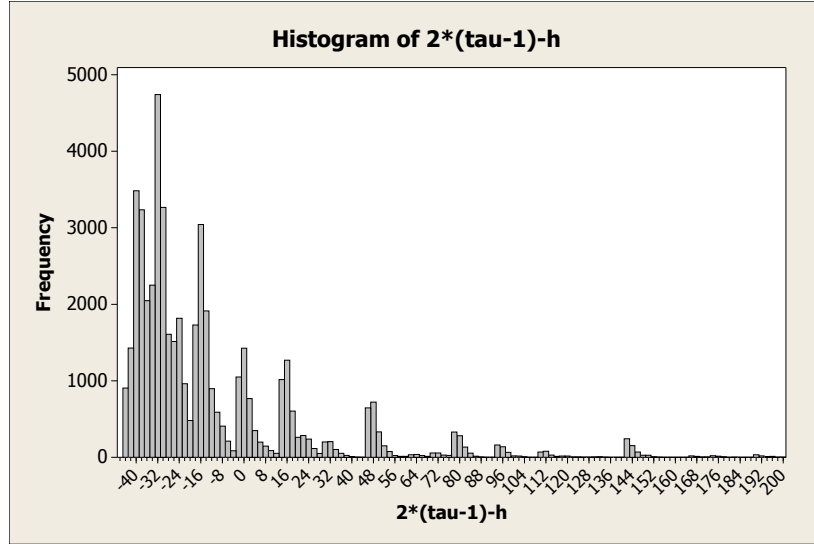


Fig. 7. Frequency histogram of $2(\tau(n - 1) - 1) - h(n)$
min = -44.96 , max = 714.41 (443 values omitted)

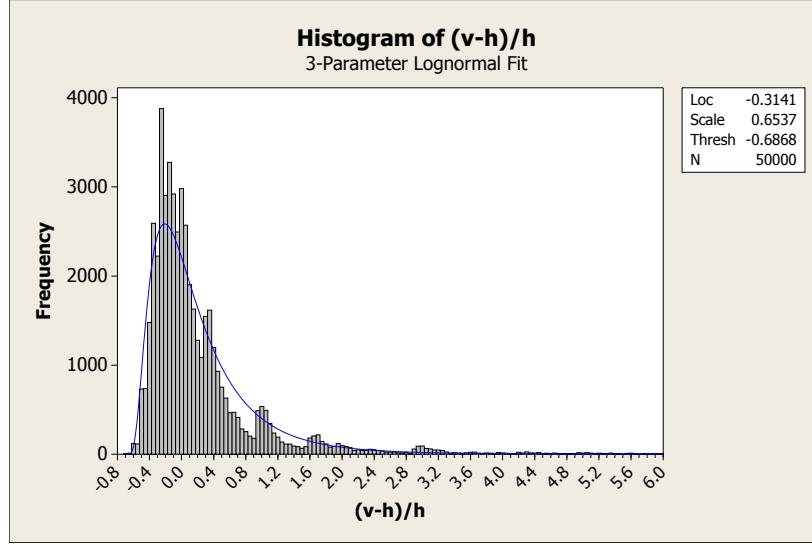


Fig. 8. Frequency histogram of $(v - h)/h$ with a lognormal fit
min = -0.68 , max = 14.77 (170 values omitted)

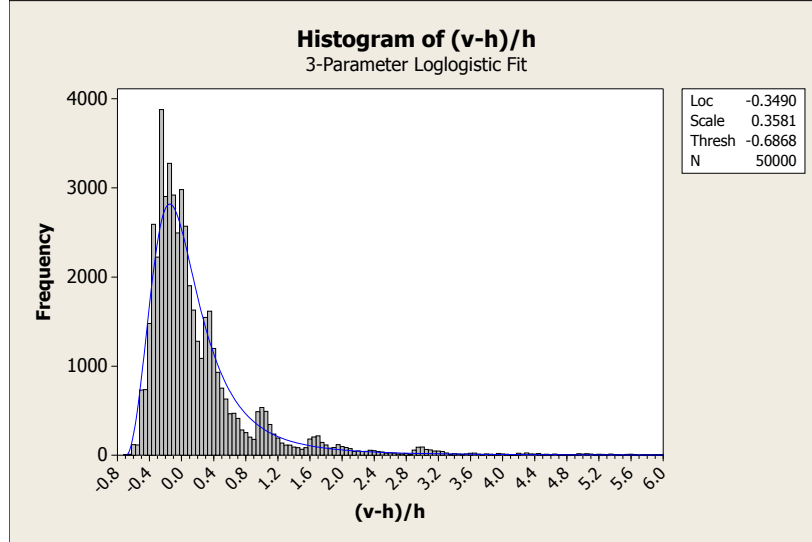


Fig. 9. Frequency histogram of $(v - h)/h$ with a loglogistic fit
min = -0.68 , max = 14.77 (170 values omitted)

The histogram in Figures 6, 8, and 9 provides evidence that for most values of n , $h(n)$ is a good approximation to $v(n)$. This leads to the main peak. After comparing the histograms in Figures 6 and 7, it is plausible to speculate that some of the secondary peaks of $(v(n) - h(n))$ to the right of 0

correspond to large values of $\tau(n-1)$ that are quite “popular”. It would be very interesting to find (at least heuristically) a right model which describes these secondary peaks (their height, frequency and so on).

Let X be a random variable. We say that X is *lognormally* distributed if $\log X$ is a normal distribution, and X is *loglogistically* distributed if $\log X$ is a logistic distribution. The probability density functions of the lognormal distribution is

$$f(x; \mu, \sigma) = \frac{\exp(-(\log x - \mu)^2/(2\sigma^2))}{\sqrt{2\pi}\sigma x},$$

where μ and σ^2 are the mean and variance of $\log(X)$. The probability density function of the loglogistic distribution is

$$f(x; \mu, \sigma) = \frac{\exp((\log x - \mu)/\sigma)}{\sigma x(1 + \exp((\log x - \mu)/\sigma))^2},$$

where μ is the scale parameter and σ is the shape parameter.

In Figures 8 and 9 we have provided the scaled histograms of $(v - h)/h$ with the lognormal fit and the loglogistic fit respectively, as both of them seem to be reasonable approximations. Numerically, the loglogistic fit seems to be better. However here is a heuristic argument (articulated by one of the referees) suggesting that the lognormal is more accurate. By the Erdős-Kac theorem [24, III.4.4, Theorem 8], $\omega(s)$ is normally distributed, and since $\tau(s) = 2^{\omega(s)+O(1)}$ for most integers s , we conclude that $\log \tau(s)$ is also normally distributed. Given the connection between $v(n)$ and the divisor functions, it seems reasonable to believe that a lognormal distribution is more accurate.

As a curiosity, we also mention that in the highly asymmetric histograms of Figures 6, 8 and 9 we still have $v(n) < h(n)$ in 25057 out of 50000 cases. It would be interesting to understand whether this is a coincidence, or whether there is some regular effect behind this.

Our heuristic explanation for the difference between $V(N)$ and $H(N)$ is as follows. Overall, G_n behaves as a “pseudorandom” set, but (as we observed in Theorem 6) there are some “regular points” on the convex closure arising from the divisors of $n-1$. For a typical integer n , these points have little effect, but for exceptional values of n , they make a substantial contribution to the value of $v(n)$ which is sufficient to interfere with the “pseudorandom” behavior of G_n . To see this, it is useful to recall that although for most integers we have

$$\tau(n-1) = (\log n)^{\log 2 + o(1)} = h(n)^{\log 2 + o(1)},$$

see [12, Theorem 432], on the average we have

$$\sum_{n=2}^N \tau(n-1) \sim N \log N \sim \frac{3N}{8} H(N),$$

see [12, Theorem 320]. Therefore, the contribution of $2\tau(n-1)$ from the points on the curves $\alpha_1(n)$ and $\beta_1(n)$ (see Theorem 6) is negligible compared to $h(n)$ for almost all n , but on average are of the same order as $0.75H(N)$. Thus it is plausible to assert that the values of $H(N)$ reflect only the “pseudorandom” nature of G_n , whereas the contribution of $2\tau(n-1)$ from the curves $\alpha_1(n), \beta_1(n)$ reflect certain “regular” properties of the points of G_n .

5.2 Weighted average contribution of divisors

The lower bound of Theorem 6 takes into account only the contribution from the divisors of $n-1$. It is plausible to assume that the divisors of $jn-1$, with “small” $j \geq 2$, also give some regular contribution to $v(n)$. This probably requires some completely new arguments since the contribution from such divisors is certainly not additive.

Experimenting with some weighted averages involving $\tau(jn-1)$ for “small” values of j , we have found that $g_1(n)$ and $g_2(n)$ where

$$\begin{aligned} g_1(n) &= 2(\tau(n-1) - 1) + 2 \sum_{j=2}^{\lfloor \log n \rfloor} j^{-3/2} \tau(jn-1), \\ g_2(n) &= 2(\tau(n-1) - 1) + 2e \sum_{j=2}^{\lfloor \log n \rfloor} e^{-j} \tau(jn-1), \end{aligned}$$

to be “reasonable” numerical approximations to $v(n)$.

It is too early to make any substantiated conjecture about the true contribution from the divisors of $jn-1$ with $j \geq 2$. Numerical experiments for a much broader range as well as some new ideas are needed. Nevertheless, our calculation raises the following question.

Question 16. *Are there “natural” coefficients c_j , $j = 2, 3, \dots$, and function $J(n)$, such that if we define $g(n)$ to be*

$$g(n) = 2\tau(n-1) + \sum_{j=2}^{J(n)} c_j \tau(jn-1),$$

then we have

$$V(N) \sim \frac{1}{N-1} \sum_{n=2}^N g(n)$$

as $N \rightarrow \infty$?

Clearly, if $V(N) \sim C \log N$, then the answer to Question 16 is positive, and one could then set $J(n) = 2$ and determine the value of c_2 by “reverse engineering”. However we are asking for coefficients c_j and a function $J(n)$ that can be explained by some intrinsic reasons, provided such reasons exist!

5.3 The difference $v(n) - 2(\tau(n-1) - 1)$

Another computer experiment that we ran on our random set of 50000 integers was to check the values of the difference $v(n) - 2(\tau(n-1) - 1)$. The histogram of our experiment is given in Figure 10.

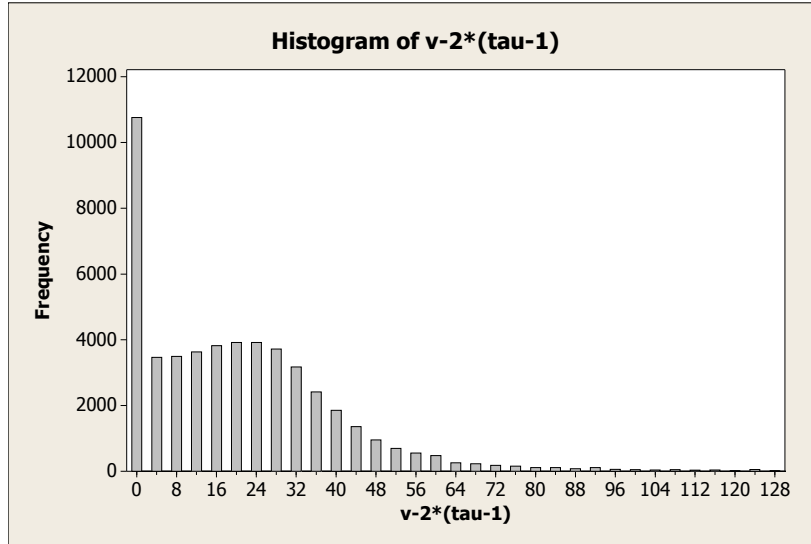


Fig. 10. Frequency histogram of $v(n) - 2(\tau(n-1) - 1)$
min = 0, max = 484 (199 values omitted)

The graph of Figure 10 suggests that the most “popular” value of $v(n) - 2(\tau(n-1) - 1)$ is 0. There is some obvious regularity in the distribution of other values which would be interesting to explain.

The way we have derived the lower bound of Theorem 6 on the frequency of the occurrence $v(n) = 2(\tau(n-1) - 1)$ from (8) raises the following question:

Question 17. Is $T(n-1) = O(1)$ for all (or nearly all) integers n with $v(n) = 2(\tau(n-1) - 1)$?

An affirmative answer to this question would then allow us to conclude that

$$\#\{n \leq x : v(n) = 2(\tau(n-1) - 1)\} \asymp \frac{x}{\log x}.$$

In our random set of 50000 integers we have 10764 integers satisfying the equality $v(n) = 2(\tau(n-1) - 1)$. For this set of 10764 integers we have computed the value of $t(n)$, where $t(n) = \lfloor (T(n-1) + 3)/4 \rfloor$. We give this histogram in Figure 11. We remark that for 7198 integers of this sample the value of $t(n)$ is 1, and for 2413 integers of this sample the value of $t(n)$ is 2. Thus for at least 9611 integers out of 10764 cases, we have $\Gamma_n \cap \alpha_2(n) = \emptyset$.

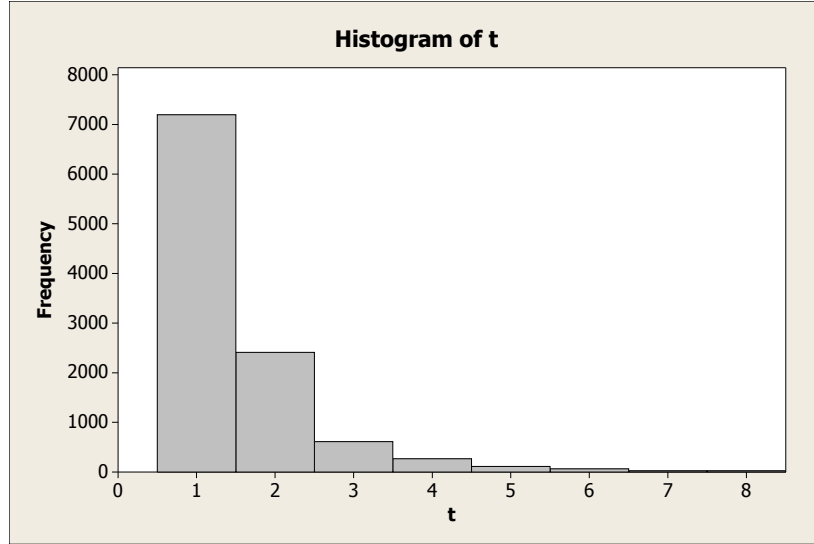


Fig. 11. Frequency histogram of $t(n) = \lfloor (T(n-1) + 3)/4 \rfloor$
min = 1, max = 26 (39 values omitted)

We have also found on examining the data that $v(n) - 2(\tau(n-1) - 1)$ is invariably a multiple of 4 and this suggests the following conjecture.

Conjecture 18. For almost all n ,

$$v(n) \equiv 2(\tau(n-1) - 1) \pmod{4}.$$

We have a simple heuristic argument for this conjecture. We know that $\tau(n-1)$ is odd if and only if $(n-1)$ is a square. Thus the conjecture reduces

to the statement that for almost all n , $4 \nmid v(n)$. On invoking Propositions 1 and 3 we have that $4 \mid v(n)$ if and only if the vertex (a_s, b_s) lies on the line $x + y = n$. *Intuitively* this seems to be a very rare occurrence (unfortunately at present we are unable to put this key remark in a rigorous context); we typically see that $a_s + b_s = n$ only when n is the shifted square $m^2 + 1$.

6 Other Curves

Studying the point sets

$$F_n(f) = \{(a, b) : a, b \in \mathbb{Z}, f(a, b) \equiv 0 \pmod{n}, 0 \leq a, b \leq n-1\},$$

where $f(X, Y) \in \mathbb{Z}[X, Y]$, is certainly a natural question, and this has been done in a number of works, see [3, 10, 25, 27] and references therein. In the case of prime modulus p , one can use the Bombieri [1] bound of exponential sums along a curve as a substitute of the bound of Kloosterman sums. In particular, for a prime $n = p$, under some mild assumptions on the polynomial f , one can easily obtain an analogue of Theorem 11 for sets $F_p(f)$. However, our other results are specific to the sets G_n and cannot be extended to other curves. It is worth remarking that for composite n , there are some analogues of the Bombieri bound, see [21], but quite naturally, they are much weaker than the bound of [1]. So the Kloosterman sums is one of very few examples where the strength of the bound remains almost unaffected by the arithmetic structure of the modulus.

Our preliminary tests show that the sets $F_n(f)$ and $F_p(f)$ have less “infrastructure” than G_n and behave more like truly random sets. For example, let $w_f(n)$ denote the number of vertices of convex hull of $F_n(f)$. We now let

$$h_f(n) = \frac{8}{3} (\log(\#F_n(f)) + \gamma - \log 2).$$

The histograms in Figures 12–14 show the relative difference $(w_f - h_f)/h_f$ for random quadratic and cubic polynomials. For the histogram of Figure 12 we chose a random value of n in the interval $[10000, 300000]$. Then based on the value of n we randomly chose the coefficients a, b, c and took $f(x, y)$ to be the polynomial

$$f(x, y) = y - ax^2 - bx - c.$$

We did this for 10000 values of n . For the histogram of Figure 13 we repeated this same experiment with random quadratic polynomials for 1000 random

primes in the interval $[7919, 611953]$. For the histogram of Figure 14 we repeated our first numerical experiment (again for 10000 values of n), but this time with random cubics

$$f(x, y) = y - ax^3 - bx^2 - cx - d.$$

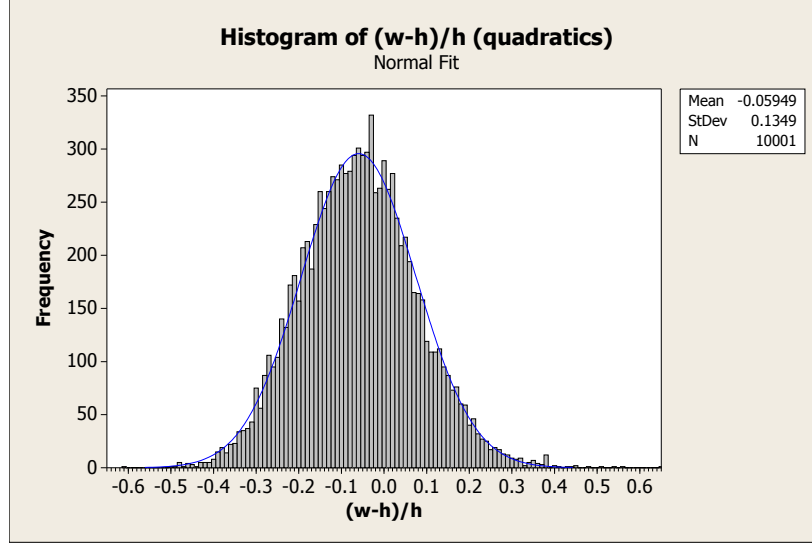


Fig. 12. Frequency histogram of $(w_f - h_f)/h_f$ for random quadratics f over random n
min = -0.607 , max = 0.65

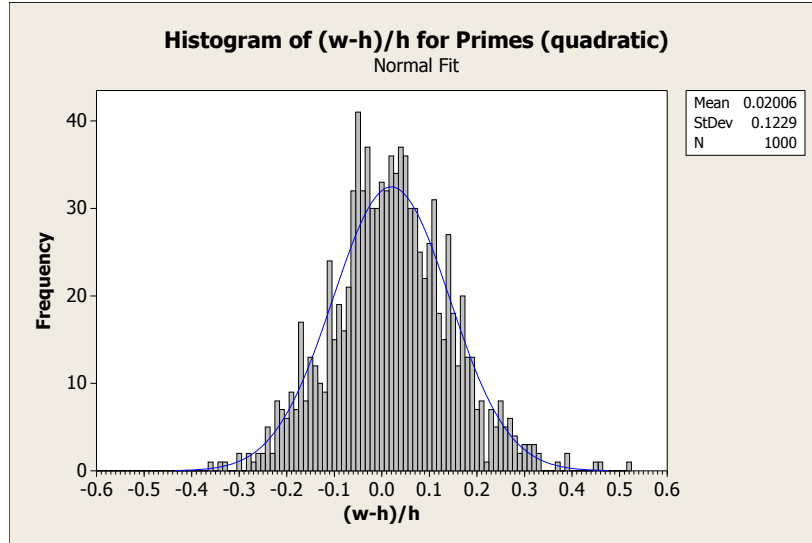


Fig. 13. Frequency histogram of $(w_f - h_f)/h_f$ for random quadratics f over random p .

$$\min = -0.355, \max = 0.518$$

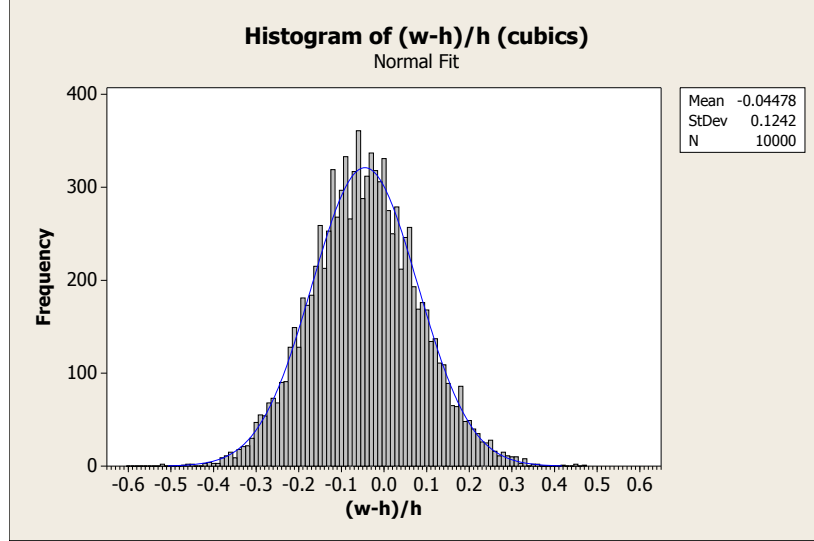


Fig. 14. Frequency histogram of $(w_f - h_f)/h_f$ for random cubics f over random n
 $\min = -0.525, \max = 0.473$

The histograms of Figures 12–14 suggest that the quantities

$$\frac{w_f(n) - h_f(n)}{h_f(n)} \quad \text{and} \quad \frac{w_f(p) - h_f(p)}{h_f(p)}$$

are both normally distributed with mean 0, and so we make the following “Erdős-Kac” type conjectures.

Let

$$\Phi_\sigma(z) = \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^z \exp\left(-\frac{t^2}{2\sigma^2}\right) dt,$$

denote the cumulative distribution function of a normal distribution with mean 0 and variance σ^2 .

Conjecture 19. *For each integer $n \geq 1$ we choose a sequence $\mathcal{F} = (f_n)$ of polynomials $f_n(x, y) \in \mathbb{Z}_n[x, y]$ of a fixed degree $d \geq 2$, chosen uniformly at random over the residue ring \mathbb{Z}_n and let*

$$\begin{aligned} \sigma_{\mathcal{F}}(N) &= \sqrt{\frac{1}{N} \sum_{n \leq N} (w_{f_n}(n)/h_{f_n}(n) - 1)^2}, \\ \rho_{\mathcal{F}}(N) &= \sqrt{\frac{1}{\pi(N)} \sum_{p \leq N} (w_{f_p}(p)/h_{f_p}(p) - 1)^2}. \end{aligned}$$

Then for any real z ,

$$\frac{\#\{n \leq N : (w_{f_n}(n) - h_{f_n}(n)) / h_{f_n}(n) \leq z\}}{N\Phi_{\sigma_{\mathcal{F}}(N)}(z)} \rightarrow 1,$$

$$\frac{\#\{p \leq N : (w_{f_p}(p) - h_{f_p}(p)) / h_{f_p}(p) \leq z\}}{\pi(N)\Phi_{\rho_{\mathcal{F}}(N)}(z)} \rightarrow 1,$$

with probability 1 (over the choice of $\mathcal{F} = (f_n)$) as $N \rightarrow \infty$.

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- The referees for their careful reading of the article. The manuscript substantially benefited from their comments. In particular we are indebted to the referee who suggested using the result of Saias [18] to show that

$$\#\{n \leq x : v(n) = 2(\tau(n-1) - 1)\} \gg \frac{x}{\log x}.$$

- Kevin Ford for suggesting the set $\mathcal{A}(x)$ that arises in the proof of Theorem 8.
- Daniel Sutanlyo for computing $\psi(3/4)$.
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